The status role of modeling and simulation in materials science and engineering

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Summary
Four materials modeling and simulation topics have been reviewed. Dislocation modeling shows significant progress in using the results of atomistic dislocation interaction calculations as input to discrete dislocation models, which, in turn, are now able to predict stress-strain relationships. Atomistic models have now been used to predict dynamic and microstructural effects on fracture. Continuum solidification models are now able to predict microstructural features. Plasticity models have been formulated that include dislocation and grain size distributions.

Introduction
The field of modeling and simulation in materials science and engineering is extremely broad and even for a single year the number of papers published is in the thousands. Since the field is so broad, I have chosen to limit the discussion in this review to four topics of great current interest in materials science and engineering: dislocations, fracture, plasticity, and liquids. In these areas I have chosen a very few papers that I feel are the most important contributions. The connection between the four areas is microstructure, which is really the essence of materials science and engineering. For metals and alloys both solidification and deformation are instrumental in producing microstructure. In the case of solidification, it is the nucleation and growth of the solid phase, while in deformation, it is the motion, interaction, and trapping of dislocations, that determines the final microstructure. Of course, it is this very microstructure that controls the fracture and plasticity behavior of these materials.

I have also limited this review to models of, what I call, ‘real’ materials, in contrast to model materials, because I feel that the goal of computational materials science and engineering is the prediction of engineering material properties. My definition of a ‘real’ material is a pure metal or engineering alloy whose basic properties e.g., elastic moduli, cohesive energy, defect energetics, are captured in the model. In contrast I consider a model material as a generic entity, e.g., an FCC or BCC material or a Lennard-Jones solid. In my opinion calculations of

model materials, although useful for understanding general mechanisms, will not lead to predictive models of complex materials.

In each of the topic areas the modeling and simulation occur at differing spatial scales e.g., atomistic modeling at the nm scale, microstructural modeling at the μm scale, and engineering modeling at the continuum level. Throughout the review I will try to point out the connections between the different size scales and how one set of calculations can be used at the next larger size scale to eventually develop a predictive model of mechanical behavior.

Dislocation models and simulations

Elasticity theory is an excellent representation of dislocation interactions at distances greater than a few Burgers vectors. Two and three dimensional elastic models of multiple dislocations are now relatively easily implemented on large computers. However, as dislocations approach each other, core overlap effects take place. In order to quantify these effects, atomistic calculations are necessary. The following recent papers show how these short-range atomistic effects are incorporated into the dislocation dynamics and also how the atomistic effects are calculated.

Rhee *et al.* [**1] have developed models of short-range processes e.g., dislocation annihilation, formation of jogs, junctions, and dipoles, and of cross slip. The bases of these short-range interaction models are critical force or angle criteria. The cross slip model is probabilistic and is based on thermal activation. They have implemented these models in a 3-D dislocation dynamics code and have calculated the stage I stress-strain behavior of Ta. Calculations up to a few tenths of a percent strain are presented. The rate and temperature effects of the flow stress are captured through the dislocation mobility. They find that the flow stress varies approximately as the inverse square root of the mobility.

Fivel *et al.* [2] have applied their 3-D dislocation dynamics model to the prediction of plastic zone behavior in Cu during indentation. Since the exact dislocation nucleation behavior under the indenter is not known, this work uses the experimental load-displacement curve to control nucleation. Geometrically necessary dislocation loops are generated to accommodate the imposed plastic displacement of the indentation tip. The predicted dislocation microstructure after an indentation of 50 nm is compared to experiment. Both the shape and extent of the dislocations are in good agreement with the experimental TEM micrographs.

Baskes *et al.*[3] investigated the effects of stress on a Lomer-Cottrell lock (LCL) formed from the intersection of two parallel lattice dislocations. Using an EAM potential [4,5] that represents the properties of Ni extremely well, they discovered that in a constrained geometry the LCL responds to uniaxial stress by three transitions. The initial configuration of the LCL consists of two Shockley partial dislocations and a stair rod dislocation. The spacing of these dislocations from atomistics agrees extremely well with elasticity theory. The first transition occurs at 2.3% strain when one partial dislocation moves through the stair rod dislocation producing extrinsic stacking fault. At 4.8% strain a new partial dislocation is emitted from the stair rod. This partial follows the motion of the first partial turning the extrinsic fault into intrinsic fault. Finally at 6% strain the second initial partial moves through the stair rod, carrying with it another new partial dislocation leaving a region of both intrinsic and extrinsic stacking fault. The final configuration is an inversion of the initial one. All of the transitions are irreversible. These calculations show that LCL evolution is extremely complicated, leading to dislocation and stacking fault generation.

Duesbery [6] used a Finnis/Sinclair potential [7] for Cu [8] to investigate cross-slip. He finds that the classical model of cross-slip, which assumes that an extended dislocation cannot leave its slip plane until it is fully constricted, is incorrect. The atomistics show that cross-slip is possible at any partial dislocation separation if the driving stress is large enough. The calculated stress for cross-slip for a fully constricted (unconstricted) dislocation is 0.023 (0.06) of the shear modulus. These stresses are equivalent to the strains calculated by Baskes *et al.*[3] for the LCL transitions discussed above.

Fracture simulations

Fracture at the continuum level is traditionally described by linear elastic fracture mechanics. However crack tip processes, which occur at an atomic level, are important in determining tradeoffs between brittle and ductile behavior or high strain rate effects. The next set of papers addresses these issues.

Miller *et al.* [**9] have applied the quasicontinuum model [10] to the fracture of Ni. This model treats atoms at a crack tip or dislocation core through EAM [11] interactions, but atoms in a homogeneous environment are lumped together to reduce the number of degrees of freedom that must be considered. In this work both a crack in a single crystal and near a grain boundary were studied. In the single crystal two orientations were presented in mode I loading, one which failed in a brittle manner by cleavage and one

which emitted dislocations. The results were compared to the unstable stacking fault model of Rice [12]. The Rice model predicts dislocation emission in both orientations, in contrast with the atomistic calculation, and in the ductile orientation, underestimates the energy release rate by 50%. For a crack near a grain boundary a number of interesting deformation mechanisms were found: the grain boundary moves toward the crack as it approaches; dislocations are emitted from the grain boundary; and the crack is arrested by the boundary leading to grain boundary sliding.

Ludwig and Gumbsch [*13] have studied the effect of loading conditions on fracture in NiAl (B2) using EAM potentials [14]. In these calculations the FEAt technique [15] is used to provide the boundary conditions for the atomistic region. By looking at a number of orientations and loading conditions, the authors conclude that perfect cleavage occurs on only the {110} crack plane in agreement with experiment. The calculated critical stress intensity factor of 0.7 MPa $m^{1/2}$ is about a factor of five smaller than experiment. Only emission of <001>{110} dislocations was observed. This emission occurred at a constant applied shear stress intensity on the glide plane. In contrast to the case of Ni above, the dislocation emission criterion is in good agreement with the Rice model [12] perhaps due to the specific orientations studied here. For the (001)[100] crack system a zig-zag crack path with surface energy higher than (001) is found. This result is in apparent conflict with the results of Farkas [16] who, using an EAM potential [17] in the same orientation, found that 1/2<111>(10-1) dislocations were emitted from the crack tip. These dislocations stayed in the vicinity of the crack tip and facilitated crack branching and cleavage along {101} planes. These effects occur at stress intensities considerably higher than those investigated by Ludwig and Gumbsch [*13] presumably due to the higher (110) surface energy in the potentials used by Farkas.

Machová and Ackland [18] studied mode I impact loading of a micro-crack in Fe using a Finnis-Sinclair potential [19]. Large models in a 2-D geometry are used to eliminate the problem of wave reflection from boundaries. The results indicate that micro-crack initiation can be treated according to linear fracture mechanics concepts. Due to the shock loading, crack extension occurs at stresses greater than about half of the Griffith stress. The dominant process at the growing crack tip is found to be transient twin formation. As the crack proceeds these twins are destroyed and crack-tip shielding dislocations appear at low crack velocities. At higher velocities the twins are again generated. In general it seems that dislocation formation is favored at low strain rates while twin formation is favored at high strain rates.

Plasticity modeling
The plastic behavior of metals is an important phenomenon in materials science and engineering. Typically modeling in this area has been very empirical with little connection to microstructural concepts. Fortunately the field is changing rapidly with connection to material microstructure and realistic micro-mechanical models becoming more common. The following two papers show how microstructural features may be incorporated into plasticity models.

Estrin et al. [*20] have developed a dislocation-based model of large strain deformation of cell forming materials. The model is based on the microstructural concept of dislocation cell formation [21], which produces a non-uniform dislocation distribution localized in the cell walls. The model is applied to torsion in Cu. This unified model reproduces stage II-V strain hardening. Both strain rate and temperature effects on hardening and dislocation densities are in agreement with experiment. In contrast to previous assumptions, the dislocation density in the cell interiors was not zero, but small, a factor of 10-35 lower than in the cell walls. The experimentally observed decrease in the volume fraction of cell wall with strain was found to be important in stage IV-V hardening.

Masumura et al. [22] developed a phenomenological microstructural based model of yield stress for ultra-fine grained material. The model included a complete grain size distribution, rather than only the average grain size. Small grains deformed by the Coble creep mechanism, while large grains obeyed the classical Hall-Petch relationship, i.e., dislocation glide plasticity. A critical grain size characterized the switch between the two mechanisms. The five parameter model was able to fit the yield stress behavior of nanocrystalline Cu and NiP.

Modeling of liquids and solid/liquid interfaces
Solidification is one of the most important phenomena in materials science and engineering. For example, it is critical in joining processes (welding, soldering, and brazing) and casting. The solidification microstructure starts the evolution towards the final microstructure, which, in turn, determines mechanical properties. Phenomenological models are frequently used to predict solidification microstructures. A key to these models is the availability of accurate thermodynamic and kinetic data. Frequently experimental data is unavailable or unobtainable. Computations are now beginning to play a role in developing a data base of properties for metals and alloys.

Warren et al. [**23] have developed a phenomenological model of the spreading of a liquid alloy on a metal substrate. Their model includes dissolution of the substrate, but not

intermetallic formation. The model predicts the dynamics of the spreading process, including the triple junction velocity, the shape of the liquid drop, and the concentration profile in the liquid. Most importantly, the diffusion boundary conditions determine the triple point motion; no additional law of motion is required. The model shows that at early times the driving force in the system is dominated by dissolution gradients (liquid thermodynamics) while at long times the driving force is controlled by curvature gradients (solid-liquid interfacial energy).

Zhao et al. [24] developed a model for the prediction of the microstructure of a hypermonotectic alloy as it is cooled through the miscibility gap. The model includes both nucleation and diffusional growth in the liquid. Predictions of the model include the number density of droplets and their size distribution as a function of cooling rate and alloy composition.

Provatas et al. [25] have developed an efficient adaptive mesh refinement method for phase field models of dendritic growth. Using mesh refinement of 2^{17}, results are presented for undercooling as low as 0.1. This method seems to have promise for allowing phase field calculations under experimentally relevant conditions.

Sasikumar et al. [*26] have developed a simple model of dendrite growth in binary alloys that presents an alternative to the phase field model [27]. The model assumes that the solid-liquid interface motion is driven by solute gradients and not by temperature gradients. Furthermore they ignore diffusion in the solid. They present dendrite microstructures that appear to represent features of actual dendrites. The model predicts that the fraction of solid in the dendritic structure is almost identical to that predicted by the Scheil equation. The authors claim that their model is capable of simulating a much larger range of cooling rate, undercooling, and grain size than the phase field model.

Alemany et al. [*28] have used atomistic MD calculations with an EAM potential [29] to calculate transport properties of Ni. Calculations were performed at two temperatures. The liquid diffusivity was found to be 3.5×10^{-9} m^2/s at 1775 K and increased slightly to 4.3×10^{-9} m^2/s at 1875 K. No experimental data was available for comparison, but these diffusivities are very similar to those measured in other liquid metals, e.g., Al-Cu or Al-Si alloys. The shear viscosity was calculated to be 4.6(3.7) mNs/m^2 at 1775(1875) K in excellent agreement with experiment 5.0(4.1). These calculations show that atomistic calculations are now at the point where reasonably accurate transport and thermodynamic properties of alloys can be predicted.

Conclusions
Modeling and simulation of materials at the atomistic, microstructural, and continuum levels continue to show progress, but prediction of mechanical properties of engineering materials is still a vision of the future. More often than not, engineering models, based on microstructural mechanisms, continue to be developed. Unfortunately, in order to gain computational efficiency, the sub-models are frequently simplified, sometimes so far that they do not capture the basic physics of the micro-mechanism. In addition simplification removes the connection to calculation of model parameters at a smaller length scale.

The paper by Rhee et al. [**1] sets a nice template for how predictive materials modeling can be accomplished. The authors formulate a number of ‘rules’ that the dislocations obey. Quantitative calculation of the ‘rules’ is now possible using atomistics and modern potentials. Using these ‘rules’ they are able to calculate the response of their multi-dislocation material to applied stress in stage I of deformation. Following this template, the continuum plasticity community should develop such a series of ‘rules’ to be used in stage II-V deformation that could be calculated by the 3-D dislocation dynamics community or obtained from experiment. These ‘rules’ would be complex, covering the interactions of groups of dislocations of various character. The object of the rules would be the connection of discrete dislocations to a spatially varying dislocation density model similar to that Estrin et al. [*20] and finally to a cell based model. If this process were accomplished, I believe that we would have a predictive model of plasticity.

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References

1. Rhee M, Zbib HM, Hirth JP, Huang H, de la Rubia T: **Models for long-/short-range interactions and cross slip in 3D dislocation simulation of BCC single crystals. Modelling and Simul. in Mater. Sci. Eng. 1998, 6:467-492.
This paper enumerates 'rules' of short-range dislocation interactions necessary for 3-D dislocation dynamics calculations. Stage I deformation in BCC Ta is modeled.
2. Fivel MC, Robertson CF, Canova GR, Boulanger L: **Three-dimensional modeling of indent-induced plastic zone at a mesoscale**. *Acta mater.* 1998, **46**:6183-6194.
3. Baskes MI, Hoagland RG, Tsuji T: **An atomistic study of the strength of an extended-dislocation barrier.** *Modelling and Simul. in Mater. Sci. Eng.* 1998, **6**:9-18.
4. Angelo JE, Moody NR, Baskes MI: **Trapping of hydrogen to lattice defects in nickel**. *Modelling Simul. Mater. Sci. Eng.*

1995, **3**:289-307.
5. Baskes MI, Sha X, Angelo JE, Moody NR: **Trapping of hydrogen to lattice defects in nickel**. *Modelling and Simul. in Mater. Sci. Eng.* 1997, **5**:651-652.
6. Duesbery MS: **Dislocation motion, constriction and cross-slip in fcc metals**. *Modelling and Simul. in Mater. Sci. Eng.* 1998, **6**:35-49.
7. Finnis MW, Sinclair JE: **A simple empirical N-Body potential for transition metals**. *Philos. Mag A* 1984, **50**:45-55.
8. Ackland GJ, Thetford R: **An improved N-body semiempirical model for body-centered cubic transition-metals**. *Philos. Mag. A* 1987, **56**:15.
9. Miller R, Tadmor EB, Phillips R, Ortiz M: **Quasicontinuum simulation of fracture at the atomic scale. *Modelling and Simul. in Mater. Sci. Eng.* 1998, **6**:607-638.
Using the quasicontinuum and an EAM potential for Ni, this paper considers the behavior of a crack tip in bulk material and near a grain boundary. Grain boundary motion and dislocation emission from the grain boundary are seen.
10. Tadmor EB, Ortiz M, Phillips R: **Quasicontinuum analysis of defects in solids**. *Philos. Mag. A* 1996, **73**:1529-63.
11. Daw MS, Foiles SM, Baskes MI: **The embedded atom method: a review of theory and applications**. *Mater. Sci. Rep.* 1993, **9**:251-310.
12. Rice JR: **Dislocation nucleation from a crack tip: an analysis based on the Peierls concept**. *J. Mech. Phys. Sol.* 1992, **40**:239.
*13. Ludwig M, Gumbsch P: **Cleavage fracture and crack tip dislocation emission in B2 NiAl: an atomistic study**. *Acta mater.* 1998, **46**:3135-3143.
This paper reports the effect of loading conditions on fracture in NiAl modeled with an EAM potential. Perfect cleavage occurs only on {110} planes in agreement with experiment.
14. Ludwig M, Gumbsch P: **An empirical interatomic potential for B2 NiAl**. *Modelling Simul. Mater. Sci. Eng.* 1995, **3**:533-42.
15. Kohlhoff S, Gumbsch P, Fischmeister HF: **Crack-propagation in bcc crystals studied with a combined finite-element and atomistic model**. *Philos. Mag. A* 1991, **64**:851.
16. Farkas D: **Fracture toughness from atomistic simulations: brittleness induced by emission of sessile dislocations**. *Acta mater.* 1998, **39**:533-36.
17. Farkas D, Mutasa B, Vailhe C, Ternes K: **Interatomic potentials for B2 NiAl and martensitic phases**. *Modelling Simul. Mater. Sci. Eng.* 1995, **3**:201-14.
18. Machová A, Ackland GJ: **Dynamic overshoot in a-iron by atomistic simulations**. *Modelling Simul. Mater. Sci. Eng.* 1998, **6**:521-542.
19. Ackland GJ, Bacon DJ, Calder AF, Harry T: **Computer-simulation of point-defect properties in dilute Fe-Cu alloy using a many-body interatomic potential**. *Philos. Mag. A*

1997, **75**:713.
*20. Estrin Y, Toth LS, Molinari A, Bréchet Y: **A dislocation-based model for all hardening stages in large strain deformation**. *Acta mater.* 1998, **46**:5509-5222.
A dislocation-based model of Stage II-V deformation in FCC materials is developed. The model is applied to torsion in Cu and agreement with experiment is found.
21. Hansen N, Kuhlmann-Wilsdorf D: **Low-energy dislocation-structures due to unidirectional deformation at low-temperatures**. *Philos. Mag. A* 1986, **64**:141-161.
22. Masumura RA, Hazzledine PM, Pande CS: **Yield stress of fine grained materials**. *Acta mater.* 1998, **46**:4527-4534.
23. Warren JA, Boettinger WJ, Roosen AR: **Modeling reactive wetting. *Acta mater.* 1998, **46**:3247-64.
A phenomenological model of the spreading of a liquid alloy, including substrate dissolution is developed. The model is applied to the Bi-Sn system.
24. Zhao JZ, Ratke L, Feuerbacher B: **Microstructure evolution of immicible alloys during cooling through the miscibility gap**. *Modelling Simul. Mater. Sci. Eng.* 1998, **6**:123-39.
25. Provatas N, Goldenfeld N, Dantzig J: **Efficent computation of dendritic microstructures using adaptive mesh refinement**. *Phys. Rev. Lett.* 1998, **80**:3308-11.
*26. Sasikumar R, Jacob E, George B: **Simulation of dendrite growth in binary alloys**. *Scripta Mater.* 1998, **38**:693-701.
A simple model of dendrite growth in binary alloys is presented. Dendrite structures under various cooling rates,undercooling, and grain size are presented.
27. Kobayashi R: **Modeling and numerical simulations of dendritic crystal-growth**. *Physica D* 1993, **63**:410-423.
*28. Alemany MMG, Rey C, Gallego LJ: **Computer simulation of the dynamic properties of liquid Ni using the embedded-atom model**. *Phys. Rev. B* 1998, **58**:685-693.
Transport properties in liquid Ni described by an EAM potential are calculated. Calculated values of the shear viscosity as a function of temperature are in good agreement with experiment.
29. Voter AF, Chen SP: **Accurate interatomic potentials for Ni, Al, and Ni_3Al.** in *Characterization of Defects in Materials,* Siegel RW, Weertman JR Sinclair R. Pittsburgh, PA:MRS; 1987:175.